1 Structure and evolution of protoplanetary disks, chemical evolution, gas-dust interactions

A. Context and state of the art

Protoplanetary disks are thin gas structures surrounding young stars in which take place the whole process of planet formation from dust growth to accretion of gas on giant planets. To understand the origin of planets the first step has to be the study of the growth of solids from the sub-micrometre dust of young protoplanetary disks (Johansen et al. 2014) and the evolution of these disks over the timescale of planet formation.

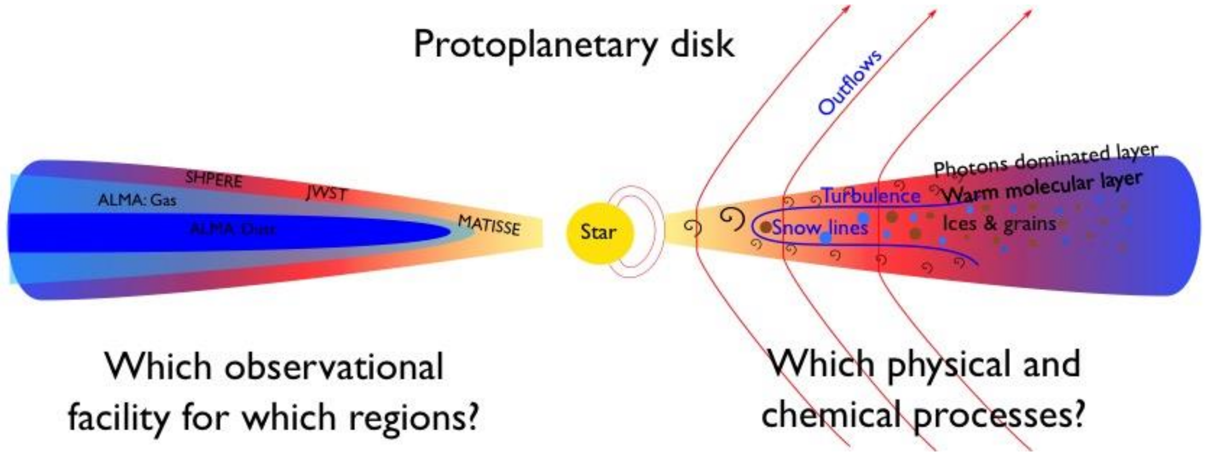

Figure A1.1: Schematic view of a vertical slice of protoplanetary disk showing which region will be probed by which observational facility (left) and some of the physical and chemical process at work in these planet forming disks.

This project is timely to achieve such a goal, as we currently have a convergence of expertise from theory to observation on these questions. On the one hand, several instruments give us more and more details on the structure of the protoplanetary disks. The ALMA observatory, which operates in submilimeter wavelength, revolutionizes our view of the concentration of dust down to the midplane of these disks. These first observations opened many questions related to the dust dynamic, the coupling of the gas with the dust and the temperature profile, which is directly related to the position of the snow lines. The SPHERE instrument results demonstrate that large-scale structures, such as spirals, warps or blobs, are present in most of the observed disks (e.g. Garufi et al. 2016). The forthcoming step for giving observational constraints for planetary formation will come from the MATISSE instrument presented in Theme 2. On the other hand, thanks to the important growth of High-Performance Computing (HPC) facilities (Theme 12.2), the theorists were able to give a completely new view on the structure of local dynamical processes at work in the different regions of the disks. Whereas it was thought until recently that the disk was mostly turbulent due to an MHD instability (MRI), the inclusion of non-ideal effects such as Hall effect and ambipolar diffusion in the simulations showed that the major part of the disk are not MRI (Simon et al. 2015). New processes have to be taken into account to understand the long-term evolution of the planetary formation regions under alternative MHD effects, such as the outflows (disk winds).

B. Current activity

Turbulence

We have performed local simulations (in the shearing-box model) of the turbulent state due to the magneto-rotational instability (MRI). This showed for the first time that this turbulence, if present in the full disk, is strong enough to explain the long-term evolution of protoplanetary disk and their lifetime. Indeed, the Reynolds and Maxwell stress associated with this turbulence do converge at a low values of viscosity to resistivity ratio, as the ones expected in the planet formation regions.

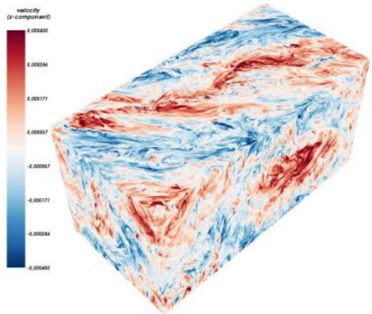

Fig. A1.2 Velocity field in a turbulent protoplanetary disk.

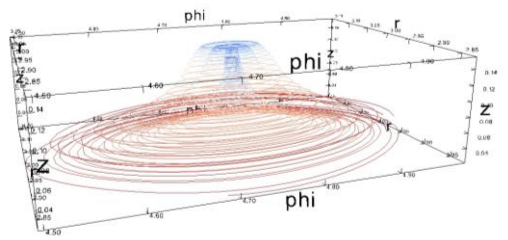

Fig. A1.3 Velocity field lines in a 3D votex

Planetesimals formation: vortices

The growth of solid of milimeter or centimetre size is a key question for planet formation. The answer will certainly involve the partial coupling between the gas and the solid. We studied the concentration of this dust by large-scale gaseous vortices and showed that up to the mass of Mars can be trapped in such structures. This result is of particular interest as similar large-scale structures have been detected by the ALMA interferometer in protoplanetary disks (van der Marel, 2013).

Temperature & Chemistry

We simulate that formation on interstellar/circumstellar ices in the laboratory. We detect amino acids (Munoz Caro et al. 2002) and other organic molecules such as aldehydes (de Marcellus et al. 2015) and simple sugars (Meinert et al. 2016) in the room-temperature residues. The formation of organic molecules (including the formation of the first carbon-carbon and carbon-nitrogen bonds) is assumed to occur in those ices and this formation is strongly temperature dependent.

Outflows

We also consider the different process at the origin of the transport of gas through the disk down to the central object. The main difficulty is to explain the conservation of angular momentum while part of fluid is falling onto the star (Turner et al. 2014). We studied if it is possible for a wind to be ejected from the disk removing part of the angular momentum, and showed that a turbulent disk can be at the origin of such wind when a vertical magnetic field is present.

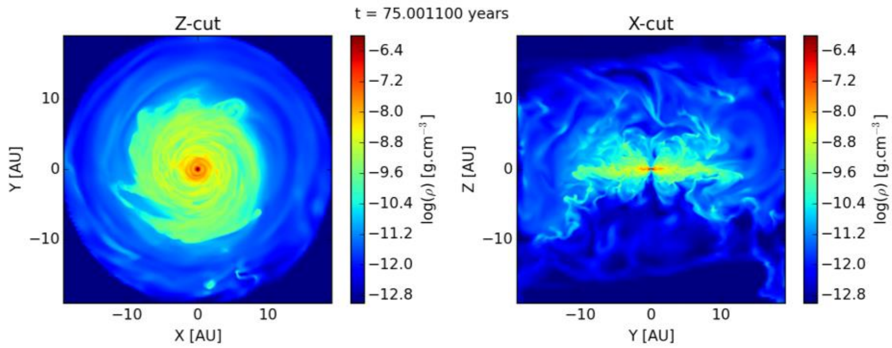

Fig. A1.4 Density in the midplane and a vertical slide of a turbulent protoplanetary disk with a vertical magnetic field.

Global disc structure

Using global simulations with a prescribed viscosity we have studied the structure of discs in which we take into account the radiative transfer and the heating by the central star. We simulate vertical slices of the disc assumed axisymmetric considering both an equilibrium disc and accretional discs at various stages of their evolution. Precisely, viscous heating dominates in the inner part of the discs while including stellar heating leads to a flared disc profile in the outer part of the disc. The transition shifts inward with time, as discs become less and less massive. A main ingredient in determining the disc structure appears to be the opacity. If the opacity depends on the local density and temperature several bumps appear in the aspect ratio of the discs. These bumps are very important as they can shield the outer disc from the stellar irradiation and they play a fundamental role in planetary migration (see Theme 6.2).

At present, we collaborate with a Japanese group on the evolution of proto-planetary disks with winds. Preliminary results suggest that the addition of disk winds could change drastically the disk profile, especially in the inner few AU.

Comparison with observations

In order to compare our understanding of the dynamics of disks and the first stages of planetesimals formation, we produced synthetic images based on our numerical simulations. The outputs of our fluid code AMRVAC were used as input of a radiative transfer code MCFOST. The results were used for successful ALMA observational time proposal of disks presenting lopsided structures similar to the ones expected when a vortex is present.

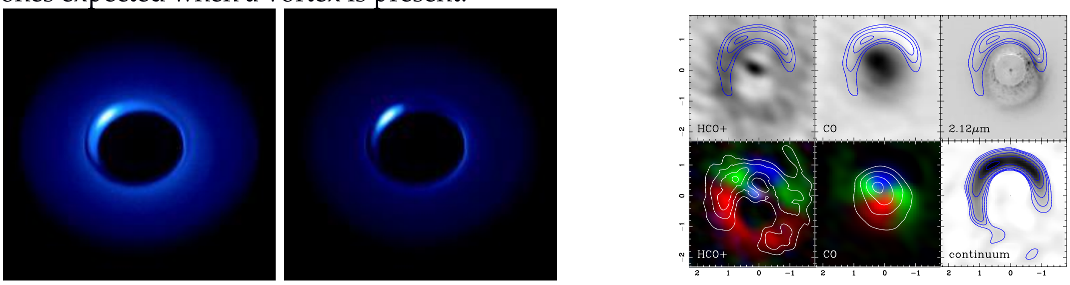

Fig. A1.5 Comparison between the synthetic images from our fluid simulation (right) and ALMA observations (Cassasus et al. 2013)

C. Future steps

Interaction between small-scale gas dynamics, vortices and MHD winds

We plan to use our expertise both on small-scale dynamics and large scale structures to study the coupling between these two key processes at work in protoplanetary disk. We are especially interested in the regions at the interface between a laminar and a turbulent flow where vortices are expected to grow. Both the small-scale gas dynamics and the large-scale magnetic structures may be at the origin of a wind, whereas the vortices have been proposed as the origin of collimated jets. These regions are then certainly central for our understanding of the evolution of the planet forming disks.

Planetesimals growth in a turbulent flow

The main difficulty in understanding the growth of intermediate size solids (mm to cm size) is to have a good description of their relative velocity. Whereas we have good simulations of the dynamic of the gas at the scale of the Astronomical Unit or the scale height of the disk, the processes at work for the growth of solids are collisions at the scale of the solid sizes. In order to present a good description of the solid growth, we need a better model of the solids velocity dispersion in the small-scale gas dynamics. Whereas this small-scale dynamics of the gas was for long considered to be due only to the magneto-rotational instability, this is not the case anymore, and we will also consider the streaming instability. We will use our expertise in turbulence and model of solids, to couple these two approaches and to propose an understanding of the dispersion of the collision velocity of micrometer to cm-size dust.

Disc thermal structure

We will implement in our codes an equation found by Price & Laibe (2014) which allows to track the dust to gas ratio in the disk for a small computational cost. This takes into account the drift and sedimentation of the dust, and the tendency of the dust to converge towards pressure maximums in the disk. Adding the dust evolution in our simulations will open great possibilities. As soon as we can follow the evolution of the gas to dust ratio in our disks, we will have a realistic and time evolving distribution of the opacity of the disk. This allows to compute the thermal structure of the disk, and produce more realistic migration maps than before (see Theme 6.2). Indeed, in the previous works, a uniform and constant dust to gas ratio of 1% was always assumed. However, it is well known that dust sediments, drifts, and grows. We must check how this influences (i) the evolution of the disk, and (ii) the migration maps.
It should be noted that the density and temperature profiles of the disks will soon be constrained with great precision by observations involving ALMA or MATISSE for instance. Most of these observations actually trace the dust distribution and not gas. The dust to gas ratio is therefore a critical parameter, and simplistic assumptions are not enough anymore.

Temperature and chemistry

We will systematically investigate chemical processes (including organic chemistry, photochemistry, stereochemistry, and chemical kinetics) that accompany disk formation and evolution. We will simulate interstellar/circumstellar ices and study the temperature dependence of the formation of first carbon-carbon bonds and the synthesis of organic molecules. Samples will be analysed by a GCxGC/TOF-MS instrument (Meinert et al. 2012). Further steps will allow us to systematically investigate the chirality of the formed organic molecules (Meierhenrich 2008).

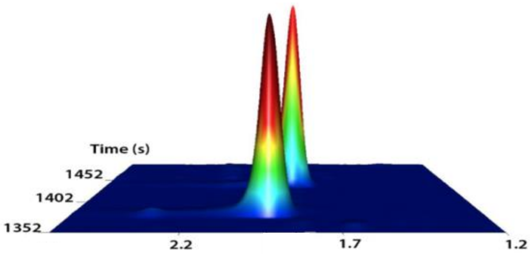

Figure. Multidimensional gas chromatogram depicting enantiomers of the amino acid alanine as identified in simulated pre-cometary ices (de Marcellus et al. 2011). L-alanine is the signal on the left, D-alanine on the right. Each point in this 3D-plot is accompanied by its mass spectrum. Mass spectra for both enantiomers are identical.

Comparison with observations

Whereas a first step has been done in the direction of the coupling of numerical fluid model of disk with observational constraints, we need to go further in this direction to have a full pipeline from the gas disk parameters to the synthetic images. In order to interpret the data from the MATISSE instrument, this pipeline will need to be extended to infrared wavelength.

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E. List of people involved in the project

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F. Most significant publications of the team

R. Miranda, D. Lai and H. Méheut. Rossby wave instability and long-term evolution of dead zones in protoplanetary discs, MNRAS, 457, 1944 :1957, April 2016
H. Meheut, S. Fromang, G. Lesur, M. Joos and P. Y. Longaretti. Magne- torotational turbulence in the small Pm limit, A&A, 579: A 117-128, July 2015
H. Meheut, Z. Meliani, P. Varniere, and W. Benz. Dust-trapping Rossby vortices in protoplanetary disks. A&A, 545 :A134-144, Sept. 2012.

Short CV of participants

H. Méheut, is an expert of turbulence and dust trap in protoplanetary disk. After a post-doc in Switzerland on planetesimal formation and at CEA Saclay on turbulent flows, she has recently been recruited at Observatoire de la Côte d'Azur as chargée de recherche.

Cornelia Meinert studied chemistry at the Universities of Rostock and Leipzig. After receiving her PhD at the Helmholtz Centre for Environmental Research by Dr. Werner Brack, she became a postdoctoral research fellow at the University Nice Sophia Antipolis, where she studied the asymmetric photolysis of amino acids and used GCxGC techniques for the enantioselective analysis of cometary and meteoritic matter. In 2013, she became a Chargé de Recherche of the CNRS. Her current research focuses on the origin of the homochirality of biomolecules.

Uwe J. Meierhenrich studied chemistry at the Philipps University of Marburg. After completing his PhD at the University of Bremen by Prof. Wolfram Thiemann, he identified amino acids in artificial comets at the Max Planck Institute for Solar System Research in Gçttingen and at the CBM in Orléans in preparation for the Rosetta cometary mission. He is now professor 'classe exceptionnelle' at the University of Nice Sophia Antipolis. He was awarded the Horst Pracejus Prize by the GDCh in 2011 for his work on chirality and enantioselective chromatography.